Appendix G: Fate and Transport Model for DW and Ohio Analyses

Introduction

EPA used a simplified fate and transport model to quantify the fate and transport of MP&M pollutant releases to surface waters in the drinking water and Ohio analyses. This model estimates pollutant concentrations at the initial point of discharge and below the initial discharge ***reach***.

The national MP&M analysis considered pollutant concentrations only at the point of discharge (see Appendix E.2.2). The drinking water and Ohio analyses account for the in-stream concentrations of pollutants at the initial point of discharge and in reaches downstream from the initial discharge reach.

This appendix describes the equations characterizing the model, its underlying assumptions, and the data sources used in model estimation. EPA combined the equations defining the model with geographic information (reach flow, velocity, length, etc.) to estimate pollutant concentrations at the initial point of discharge and below the initial discharge reach.

The estimation of pollutant concentrations below the initial discharge reach includes several factors that reduce the in-stream pollutant concentrations with the passage of time. These factors include: ***volatilization***, ***sedimentation***, and chemical decay from ***hydrolysis*** and ***microbial degradation***. EPA adjusted concentrations for changes in stream flow volume in downstream reaches. The discussion below outlines the main assumptions of this analysis. Although more advanced models are available that account for time-variable flow, sediment transport, channel geometry changes within a reach, and detailed simulation of all in-stream processes, these models will not necessarily produce more accurate results without sufficient data to support the input parameters. Estimates of the input parameters required by these models are subject to a high degree of uncertainty when applied on a national scale, and gathering such data is beyond the scope of this study.

EPA has previously applied the approach used in this analysis. For example, the first-order contaminant degradation relationship described below in Equation G.1 is currently being used by the Office of Pollution Prevention and Toxics for exposure analysis in the ReachScan computer program.

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G.1 Model Equations

The total pollution concentration in the water columns for each reach included in the analysis is calculated by the following equation expressed in generic terms of mass (M), length (L), and time (T):

$$C_T = \frac{W_T}{Q} x\, e^{\left[-\left(\frac{V_T}{H}\right)\left(\frac{x}{U}\right)\right]} \qquad \text{(G.1)}$$

where:

C_T = total toxicant concentration in the water column (M/L^3),
W_T = mass input rate of toxicant (M/T),
Q = river flow (L^3/T),
V_T = overall net loss rate of chemical (L/T),
H = flow depth (L),

x = distance downstream from the point of release (L), and
U = flow velocity (L/T).

In reaches where more than one facility is discharging, or where pollutant loadings occur from upstream reaches, the mass input rate (W_T) represents a combined input rate from all relevant industrial facilities affecting the reach. The relevant industrial facilities in the drinking water risk analysis are all MP&M sample facilities (see Chapter 13). The relevant industrial facilities in the Ohio case study analysis include:[1]

- all sample MP&M facilities,
- non-sample MP&M facilities, and
- non-MP&M facilities.

The overall net loss rate of chemical (V_T) is given by:

$$V_T = V_{Td} + V_{Ts} = (k_l + K_d{}^H) \times f_d + v_n f_p \quad \text{(G.2)}$$

where:
V_T = overall net loss rate of chemical (L/T),
V_{Td} = dissolved chemical loss rate (L/T),
V_{Ts} = loss of chemical due to sediment interaction (L/T),
k_l = volatilization transfer coefficient (L/T),
K_d = dissolved chemical decay rate (hydrolysis and microbial degradation) (1/T),
H = flow depth (L),
f_d = dissolved fraction of toxicant (unitless),
v_n = net loss of solids (L/T), and
f_p = particulate fraction of toxicant (unitless).

The dissolved and particulate fractions of the pollutant, f_d, and f_p , respectively, are estimated by:

$$f_d = \frac{1}{1 + K_p{}^S} \quad \text{(G.3)}$$

and

$$f_p = \frac{K_p{}^S}{1 + K_p{}^S} \quad \text{(G.4)}$$

where:
K_p = partition coefficient [L^3/M], and
S = suspended solids [M/L^3].

The dissolved concentration of ***metals*** and most other pollutants in the water column is generally considered a more accurate expression than the total concentrations of the toxic or bioavailable fraction. For this reason, EPA modified Equation (G.1) to express the pollutant concentrations in terms of dissolved concentration. The dissolved fraction of a pollutant is estimated as:

$$C_d = f_d \times C_T \quad \text{(G.5)}$$

Substituting equation (G.2) for C_T results in the dissolved pollutant concentration being expressed as:

[1] See Chapter 22 for detail.

$$C_d = \frac{\frac{W_T}{Q} \times e^{\left[-\left(\frac{K_d{}^H + k_l}{(1 + K_p{}^S)^H} + \frac{v_N K_p{}^S}{(1 + K_p{}^S)^H}\right) \times \left(\frac{x}{U}\right)\right]}}{1 + K_p{}^S} \quad \text{(G.6)}$$

G.2 Model Assumptions

The following three principal assumptions underlie Equation G.5:

G.2.1 Steady Flow Conditions Exist Within the Stream or River Reach

This assumption is necessary due to this study's broad geographical coverage. This assumption significantly reduces the computational effort and input parameter requirements and still produces a good first fate and transport modeling of pollutants in surface waters.

The pollutant concentration is completely mixed, both laterally (across the stream) and vertically (with depth) within each reach. The approach involves a two-dimensional model in which the concentration is uniform over the entire cross-section of the stream reach but varies with the distance of the reach. EPA assumed that the contaminant completely mixes at the point of release. This assumption will likely underestimate the concentration of a contaminant release in areas where mixing is incomplete (e.g., shore-hugging plume) and overestimate concentrations in areas beyond the point showing incomplete mixing (e.g., in areas beyond a shore-hugging plume).

G.2.2 Longitudinal Dispersion of the Pollutant Is Negligible

The model does not account for mixing outside the plane of discharge along the river reach, although it predicts variation in pollutant concentrations over distance due to both pollutant fate and decay and the differing hydrology of downstream reaches. In natural streams, longitudinal velocity gradients due to channel irregularities can cause mixing, thereby decreasing the peak concentrations as the contaminant moves downstream from the point of release. Under steady-state situations, however, the longitudinal dispersion of the pollutant is assumed to be negligible. The solution of the dispersion equation approximates a first-order decay function such as the one shown in Equations G.1 and G.5 under steady flow conditions and complete lateral and vertical mixing.

G.2.3 Flow Geometry, Suspension of Solids, and Reaction Rates Are Constant Within a River Reach

EPA assumes the data that describe a river reach and that are calculated for a reach to be constant for the full extent of the reach.

G.3 Hydrologic Linkages

EPA modeled pollutant concentrations for a distance of 500 km downstream from the discharge point in the drinking water risk analysis. In the Ohio case study analysis, EPA used the lesser of 500 km or the distance to the Ohio border from the initial discharge point to identify reaches potentially affected by pollutant discharges from this discharge point. The Agency obtained Information on the hydrologic linkages between reaches from the REACH2 file of EPA's ***Graphical Exposure Modeling System (GEMS)***. The GAGE file in GEMS provided flow (mean flow, 7Q10) and velocity (mean, low) data for each reach.

EPA used the process equations listed above to estimate both the initial pollutant concentrations at the beginning of each reach and the changes in concentrations as pollutants traveled to the end of the reach. The concentration at the end of each reach served as the value for the beginning of the next reach.

G.4 Associating Risk with Exposed Populations

The number of individuals served by each drinking water intake is an output of the fate and transport model described in this Appendix. If a drinking water intake exists on the initial reach or any downstream reach, then the model calculates the in-stream pollutant concentration at that intake. Data on the population served by the intake is saved with the concentration for further analysis (see Chapter 13 for a discussion of the cancer risk assessment).

G.5 Data Sources

Data sources used for the fate and transport model are discussed briefly in the section below, by categories of information.

G.5.1 Pollutant Loading Data Used in the Drinking Water Risk Analysis

EPA estimated annual pollutant loadings (kg/yr) for the direct and indirect sample MP&M facilities analyzed under the various regulatory options. The Agency first adjusted pollutant loadings for indirect dischargers to reflect POTW treatment, and then divided annual pollutant loadings by the number of days in one year (365) to establish daily pollutant loadings.

G.5.2 Pollutant Loading Data Used in the Ohio Case Study Analysis

EPA estimated pollutant discharges from both MP&M and significant non-MP&M sources at the reaches included in the Ohio case study analysis. Consumer perception and valuation of enhanced water-based recreational opportunities depend on the absolute level of pollutant contamination at recreation sites, and on the change in contamination from the baseline to the post-compliance cases. For this reason, capturing the effect of concurrent discharges from all MP&M and other pollutant sources is particularly important for the recreational benefits analysis.

EPA used the Office of Water's ***BASINS*** software package to identify all possible point source dischargers contributing to ambient pollutant concentrations at a given reach. BASINS is a GIS-based system that serves as a database management system for water quality monitoring, point-source pollutant discharge, and various geo-technical data. Several sources provide information on point source discharges to BASINS, including the ***Permit Compliance System*** (PCS) and ***Toxic Release Inventory*** (TRI) databases. Version 2.0 includes data reported through 1996. Preprogrammed queries in BASINS generate information on various point source discharge variables at either the state or watershed level. BASINS data on point source dischargers include:

- location information on major industrial dischargers, including PCS facilities and facilities reporting under TRI;
- SIC codes;
- flow volume; and
- discharge characteristics for up to 50 pollutants or parameters for PCS facilities.

The following sections describe steps used to characterize both MP&M and non-MP&M discharges in Ohio.

a. Characterize MP&M facility discharges

EPA used different approaches to assign discharge characteristics to MP&M facilities in Ohio, based on the level of information available for each facility. The Agency divided all MP&M facilities into three groups, based on the level of information provided by different sources:

❖ ***Facilities covered by the detailed Phase 1 and 2 questionnaire (hereafter, sampled MP&M facilities)***

The detailed surveys contain data on:

- discharge status;
- discharge volume;
- industrial processes used;
- pollution prevention activities;
- employment, revenue, and costs.

EPA engineers estimated loadings of 131 MP&M pollutants using information on facilities' processes and pollution prevention activities. All MP&M facilities in this group therefore have extensive data on their location, size, and discharge characteristics.

❖ ***Facilities covered by the detailed Iron and Steel questionnaire (hereafter sampled I&S facilities)***

The detailed I&S survey contained data similar to the detailed MP&M survey. EPA engineers used data on I&S facilities' processes and pollution prevention activities to estimate pollutant loadings from these facilities.

❖ ***Facilities covered by the Phase 2 screener questionnaire or that were covered by the Phase 1 mini-DCP (hereafter, MP&M screener facilities).***

The screener surveys contain significantly fewer data on MP&M facilities. The data collected from the screener survey recipients include:

- facility location, which can be used to assign the facilities to receiving waterways or receiving POTWs;
- SIC codes;
- discharge status (i.e., whether the facility discharges process wastewater and the approximate amount);

- employment and revenue data;
- whether the facility is engaged in manufacturing, maintenance or repairing activities; and
- data on MP&M unit operations (including type of MP&M unit operations performed at the site, and whether process wastewater is discharged as a result of each operation).

The project engineers used these data to estimate pollutant loadings for these facilities. Loading estimates for the screener facilities, which are based on less comprehensive information, involve greater uncertainty.

❖ ***Facilities that respond to neither the screener nor detailed questionnaires (hereafter referred to as non-sampled MP&M facilities)***

To address the problem of omitted discharge information on non-sampled MP&M facilities, EPA used information from the 1600 screener MP&M facilities and a random draw approach to assign the relevant characteristics for non-sampled MP&M facilities. Each screener facility represents *n* non-sampled facilities, where *n* is determined by the screener facility sample weight. All non-sampled facilities are smaller indirect dischargers because all direct MP&M facility dischargers and large indirect discharging facilities in Ohio are covered by the long, short, or screener questionnaire.

The exact location of non-sampled facilities is unknown. All non-sampled facilities discharge to one of the Ohio's POTWs because they are indirect dischargers. The Agency assigned *n* facilities represented by each screener facility to the receiving POTWs by drawing a random sample of *n* POTWs from the universe of POTWs in Ohio.[2] The Agency assigned screener facility characteristics (i.e., pollutant loadings) to all *n* facilities represented by the screener facility.

EPA used a random draw procedure for all observations from the screener survey that have a sample weight greater than one.

b. Characterize non-MP&M point source discharges

EPA used preprogrammed queries in BASINS to obtain information on all non-MP&M point source discharges in Ohio. BASINS data on non-MP&M point source dischargers include:

- location,
- SIC codes,
- flow volume, and
- discharge characteristics for up to 50 pollutants or parameters for PCS facilities.

The Agency assigned discharge characteristics to all non-MP&M industrial direct discharges based on the information provided in BASINS. POTW effluent may contain pollutants from both MP&M and non-MP&M discharges. The Agency combined information from BASINS with loading estimates provided by the project engineers to estimate total pollutant loadings from a given POTW. This analysis used the following assumptions to estimate total POTW pollutant loadings under the baseline discharge levels:

- If a POTW was not estimated to receive discharges from the MP&M facilities, then the analysis used POTW loadings reported in BASINS.
- If a pollutant or a parameter was not reported in BASINS, then the analysis used aggregate loadings from all MP&M facilities discharging to a given POTW to calculate total POTW loadings of a given pollutant.
- If a POTW was estimated to receives discharges from MP&M facilities and a given pollutant was reported in BASINS, then the analysis used the greater of the aggregate loadings from all MP&M facilities or POTW loadings reported.

EPA estimated post-compliance pollutant loadings from each POTW by subtracting the estimated reduction in the MP&M facility loadings for a given pollutant from its total baseline loadings for a given POTW.

c. Characterize nonpoint source discharges

The water quality analysis in Ohio used empirical data on ***Total Kjeldahl Nitrogen*** **(TKN)** concentrations to characterize the baseline water quality conditions. Empirical data on in-stream concentrations captured TKN contribution from both point and nonpoint sources under baseline conditions. EPA estimated changes in TKN concentrations resulting from the proposed rule by using the estimated pollutant loading reductions from MP&M sources and the water quality model described above. The Agency assumed that the non-point source contribution of toxic pollutants found in MP&M effluent to ambient concentrations of these pollutants in Ohio's streams and lakes is negligible.

[2] The Agency was unable to validate random assignments because POTWs do not know all of their MP&M dischargers. For the final rule, the Agency will perform a sensitivity analysis based on alternative draws to test the stability of the results.

GLOSSARY

BASINS: a software package that serves as a database management system for water quality monitoring, point-source pollutant discharge, and various geo-technical data, and also provides an analytic platform for modeling in-stream pollutant concentrations over an entire watershed based on multiple sources of pollutants withing the watershed. (http://www.epa.gov.OST/BASINS)

Graphical Exposure Modeling System (GEMS): A computer system designed for exposure modeling and assessment.

hydrolysis: the decomposition of organic compounds by interaction with water. (http://www.epa.gov/OCEPAterms)

metals: inorganic compounds, generally non-volatile, and which cannot be broken down by biodegradation processes. They are a particular concern because of their prevalence in MP&M effluents. Metals can accumulate in biological tissues, sequester into sewage sludge in POTWs, and contaminate soils and sediments when released to the environment. Some metals are quite toxic even when present at relatively low levels.

microbial degradation: a process whereby organic molecules are broken down by microbial metabolism.

Permit Compliance System (PCS): a computerized database of information on water discharge permits, designed to support the National Pollutant Discharge Elimination System (NPDES). (http://www.epa.gov/ceisweb1/ceishome/ceisdocs/pcs/pcs-exec.htm)

MP&M reach: a reach to which an MP&M facility discharges.

sedimentation: : letting solids settle out of wastewater by gravity. (http://www.epa.gov/OCEPAterms)

Total Kjeldahl Nitrogen (TKN): the total of organic and ammonia nitrogen. TKN is determined in the same manner as organic nitrogen, except that the ammonia is not driven off before the digestion step.

Toxic Release Inventory (TRI): database of toxic releases in the United States compiled from SARA Title III Section 313 reports. (http://www.epa.gov/OCEPAterms)

volatilization: a process whereby chemicals dissolved in water escape into the air. (http://www.epa.gov/OCEPAterms)

ACRONYMS

GEMS: Graphical Exposure Modeling System
IFD: Industrial Facility Discharge
MMR: manufacturing, maintenance or repairing activities
PCS: Permit Compliance System
TKN: Total Kjeldahl Nitrogen
TRI: Toxic Release Inventory